Scatterplots for Unordered Pairs

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ABSTRACT

Intraclass correlation coefficients (ICCs) measure the strength of the similarity among measurements within a class (or family) relative to the total variability. Classically this index of association has been most often treated as a ratio of variance components, namely the fraction of the total that the family-to-family variability represents. For the special case of twins, or any other set of unordered pairs, it is not clear which scatterplot one should use to graphically represent the ICC.

We propose that the set of all permutations within pairs of exchangeable measurements forms a legitimate basis for selecting a representative scatterplot. The recommended plot is the one whose interclass coefficient is closest to an ICC. For the product-moment version this implies that one selects a plot with r equal to the ANOVA estimator. The principle extends to other measures of association.

KEY WORDS: Graphics, Intraclass correlation, Permutation distribution, Randomization, Twins.

1. INTRODUCTION: HOW SHOULD WE PLOT TWINS?

A consultant has a client with data on identical twins, where there is no distinction in the ordering of each twin pair. The client is interested in measuring the similarity between the twins and would like a scatterplot as a visual reinforcement of this similarity. The consultant realizes that, there being no statistical difference between these siblings (they are assumed to have the same marginal distributions), the individuals within each pair are

interchangeable. With n pairs of twins, there are 2^n possible scatterplots of the points. How should the consultant plot these data? For example, Figure 1 contains a variety of such scatterplots from a small data set. If the X-Y labels are arbitrary, is one of these plots as good as another?

2. INTRACLASS CORRELATION

The measure of similarity that the client seeks has often been quantified by an intraclass correlation coefficient (ICC). The intraclass correlation, ρ, is defined to be the correlation between two individuals in the same class or family (cf. Stuart and Ord 1991, pp. 989-990). Various ICCs have been proposed for different situations. Müller and Büttner (1994) and Karlin, Cameron, and Williams (1981) give good discussions of some of these ICCs. The focus of this note is on two ICCs proposed by Fisher [1948, (first edition 1925)].

2.1 Fisher's "Symmetrical Table"

In the case of twin data, Fisher (1948) recognized the interchangeability of the twins. In motivating his treatment of intraclass correlation, he forced the estimated marginals to be equal by constructing what he called a "symmetrical table." Given n independent pairs of twins, (X_i, Y_i), $i = 1,...,n$, Fisher added n more pairs: (Y_i, X_i), $i = 1,...,n$, and computed the Pearson product-moment correlation of the $2n$ pairs. We denote this statistic by r_s (see the Appendix for more detailed notation). With this device he linked the intraclass correlation to the "interclass" coefficient. When the twins come from a bivariate normal distribution, r_s is the maximum likelihood estimate of ρ (Karlin et al. 1981).

2.2 The ANOVA Setting

Another ICC comes from the one-way random effects ANOVA model. Although Fisher did not actually use such models in his original discussion, let

$$X_{ij} = \mu + a_i + e_{ij},$$

$i = 1,\ldots,n$, $j = 1$ or 2, where μ is a constant and a_i and e_{ij} are independent random variables with variances σ_a^2 and σ_e^2, respectively. Here a_i is viewed as a family effect with σ_a^2 representing the variability among family means. Under this model the intraclass correlation is

$$\rho = \mathrm{Corr}(X_{i1}, X_{i2}) = \frac{\mathrm{Cov}(X_{i1}, X_{i2})}{\mathrm{Var}(X_{ij})} = \frac{\sigma_a^2}{\sigma_a^2 + \sigma_e^2} \geq 0.$$

The most commonly used estimate of ρ — not only for twins, but for variable family sizes as well — is

$$\hat{\rho}_A = \frac{\hat{\sigma}_a^2}{\hat{\sigma}_a^2 + \hat{\sigma}_e^2},$$

where $\hat{\sigma}_a^2$ and $\hat{\sigma}_e^2$ are the usual estimates of σ_a^2 and σ_e^2 from the ANOVA model (cf. Snedecor and Cochran 1989, pp. 242-243). It was known to Fisher that r_s is negatively biased. He went so far as to call it "slightly defective" (Fisher 1948, p. 223). In the next section we shed some more light upon this.

3. IF FISHER HAD A WORKSTATION

If Fisher had access to modern statistical computing facilities, he might have explained intraclass correlation in terms of the permutation set of all 2^n labelings of the twin pairs. For every labeling of the pairs, r_s and $\hat{\rho}_A$ remain unchanged. But which scatterplot should one use as a visual aid? Which is most "representative" of the relationship between the twins? Clearly, Fisher was of a mind to consider permutation sets, yet he may not have seen any value in discussing all of these interchangeable displays.

It seems reasonable when considering all permutations of the 2^n labelings, to choose a scatterplot whose Pearson product-moment correlation is close to an accepted measure of the intraclass correlation. It seems safe to say that the most commonly used ICC has been $\hat{\rho}_A$. Hence, it provides a reasonable benchmark for a "representative" scatterplot. It seems ironic that R. A. Fisher, an early advocate of randomization, did not discuss this permutation set — at least for calculating an ICC; if not for actually defining it.

To illustrate this idea, consider the IQ measurements on five pairs of twins in Table 1. These were randomly chosen from eight pairs of fraternal twins given by von Eye and Lienert (1980). Figure 1 shows the scatterplots and Pearson correlations, r, for half of the $2^5 = 32$ labelings of the twins. It is sufficient to consider only these, since each has a mirror image over $y = x$ with an identical value of r. Subsequently we will use r' to denote a generic value from this permutation distribution.

The coefficients range from .414 to .867 as the labeling of the twins changes. The value from Fisher's "symmetrical table," $r_s = .404$, is smaller than any of the correlations in the 16 scatterplots. For these data, $\hat{\rho}_A = .493$. The scatterplot with a correlation closest to $\hat{\rho}_A$ has $r = .497$. We would propose this as our *representative scatterplot*.

A slightly larger data set of 12 pairs of twins comes from Snedecor and Cochran (1989); originally in Newman, Freeman, and Holzinger (1937). These data, given in Table 2, are the numbers of finger ridges on both hands of female identical twins. There are $2^{11} = 2048$ relevant scatterplots; too many to examine. Instead, consider a histogram of the values of r' (Figure 2). The dashed line marks the correlation from Fisher's "symmetrical table" ($r_s = .9626$), which again is less than all of the correlations from the 2048 scatterplots. A proof of a general result to this effect can be found in the Appendix. The solid line marks the ANOVA estimate ($\hat{\rho}_A = .9656$). Figure 3 shows the scatterplot with r' closest to $\hat{\rho}_A$, as well as the scatterplots with the median (.9702), minimum (.9627), and maximum (.9890) values of r' from the permutation distribution. In light of Figure 2, the median scatterplot may also be a reasonable choice for a representative scatterplot. In this case all of the scatterplots in the permutation distribution look very similar, because ρ is apparently quite close to 1. Ultimately, the consultant may view a small sample of plots, the plot associated with the median r', or the proposed representative plot with r' closest to $\hat{\rho}_A$.

One concern, perhaps substantial, about our proposal is that Pearson's r uses neither $\hat{\mu}$, the estimate of the common mean, nor the pooled variance. Detailed notation for this model with equal marginals is in the Appendix. So, even though investigators have been viewing scatterplots for years and seeing r as the index of linear association, it does not embody the constraints that hold for twins. In other words, because r employs $\overline{X}$ and $\overline{Y}$

(and separate variances) some may argue that it is an inappropriate index. One reply to such a concern is that $\hat{\rho}_A$ is the appropriate numerical value but most investigators have visual experience with the values of r that go with patterns in graphs. That is to say, the value of $\hat{\rho}_A$ handles the model in the right way, and yet practitioners are for the most part calibrated from seeing scatterplots with a corresponding r.

4. SAMPLING THE PERMUTATION DISTRIBUTION

As the number of pairs gets moderately larger, the size of the permutation distribution becomes somewhat unmanageable. For $n = 21$, there are over one million scatterplots potentially with distinct correlations. Each addition of one more pair of twins doubles that number. For larger data sets, we must rely on sampling the 2^n scatterplots. Sampling several thousand of these is quite easy since all 2^n scatterplots are uniquely determined by the binary representation of the first 2^n integers. Hence, we only need to sample from the first 2^n integers. See Venables and Ripley (1994, pp. 144-145) for an S-PLUS function that generates the binary representation of an integer.

In our experience with simulations from bivariate normals for various values of ρ and small n, the median of the true permutation distribution of r' agrees well with $\hat{\rho}_A$. Consequently, it appears to be immaterial which of the two corresponding scatterplots is selected to be representative. This will guide us in designing a sampling procedure as an approximation when n is too large.

Enumeration is impractical whenever n is greater than about 20. Indeed most statisticians may prefer random samples to a census for $n > 11$, where there are more than 1024 candidate values of r'. We will randomly sample M scatterplots from the permutation distribution. This sample is to be searched for the value of r' closest to $\hat{\rho}_A$ or sorted to find the median. As a guideline for choosing M, the standard error of the sample median is asymptotically $\left[4nf_{r'}^2(\rho')\right]^{-1/2}$, where $f_{r'}$ is the pdf of a smooth version of the relevant permutation distribution and ρ' is its median. Rather than attempt to bound this density or even to model it as a smooth pdf, we rely upon

$$\text{Var}\left[\text{median}(r')\right] \approx \text{Var}\left[\text{mean}(r')\right] < \frac{1}{M}\text{Var}[r] \approx \frac{\left(1-\rho^2\right)^2}{Mn}. \tag{1}$$

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The inequality holds easily because the unconditional sampling distribution of r has a greater variance than from conditionally fixing the observed values and interchanging within pairs. The final approximation is from Johnson and Kotz (1970, p. 225). The similarity with Fisher's approximate $\text{Var}[\hat{\rho}_A]$ is addressed by Donner and Koval (1983). (1) suggests that we can achieve $\text{SE}[\text{median}(r')] \le d$ by choosing $M \ge \dfrac{(1-\rho^2)^2}{d^2 n}$. It is not too ambitious to set $d = .01$, because for $n \ge 20$ the worst case ($\rho = 0$) yields $M \ge 500$. This is our recommended number of subsamples from the permutation distribution, although one may refine it considerably by substituting a desired value of d and $\hat{\rho}_A$ for ρ in the inequality.

As an example we consider a data set (Table 3) concerning low density lipoprotein cholesterol (LDL–C), known to be positively associated with heart disease. The data are a subset of a larger database collected to investigate the genetic determinants of LDL–C. We gratefully acknowledge Dr. Jonathan Cohen, University of Texas Southwestern Medical Center, for allowing us to use this data which consists of LDL–C measurements (mg/dl) on 31 pairs of full brothers whose ages range from 5 to 15 years. Following fairly standard practice, ordering the siblings according to their age (x = oldest; y = youngest) yields $r = .353$, while the $\hat{\rho}_A = .362$. In the above formula for the number of representative samples required to accurately obtain an estimate of the median r', we substitute $\hat{\rho}_A$ for ρ and obtain 244 as lower bound for M. Figure 4(c) shows a histogram of $M = 301$ sample values of r'. The scatterplot associated with the median r' from this sample is shown in Figure 4(a); the median is .362 agreeing with $\hat{\rho}_A$. The latter result indicates that the scatterplot corresponding to the age ordering should be similar to that shown in Figure 4(a) and it is. In this case, the agreement is fortuitous. In general, however, arbitrarily selecting an ordering, e.g., according to age, and basing an association on the subsequent scatterplot and r may be misleading. For instance, suppose we choose to order the pairs according to the magnitude of LDL–C measurements: $x_1 = \min(x, y)$ and $x_2 = \max(x, y)$. The resulting scatterplot is given in Figure 4(b) with $r = .719$, about twice as large as $\hat{\rho}_A$.

5. PERMUTATION TEST OF INTERCHANGEABILITY

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One of the assumptions we made from the beginning was that the order of each twin pair is arbitrary. This implies that the marginal distributions are identical. Hence, we can test the hypothesis that paired data come from a distribution with identical marginals (i.e., that the pairs are interchangeable) by comparing the observed correlation to the permutation distribution of 2^n correlations. There is more to consider, but this is an important feature implied by the null; see Bradley and Blackwood (1989) for a simultaneous test on means and variances.

As an example, consider the data in Table 4 given by Müller and Büttner (1994). These data are measurements by two different observers of cardiac output of 23 patients using Doppler echocardiography. It is clear here that the order of the pairs is *not* arbitrary. One may be interested in testing whether the measurements by observer A and observer B are consistent with each other. Since the permutation distribution has more than four million correlations, we must rely upon sampling from this distribution for an approximate randomization test of interchangeability. Figure 5 shows the original scatterplot of the data, with a correlation of .924, along with 19 randomly selected scatterplots from the permutation distribution, with their correlations. Our observed correlation exceeds the correlation in all 19 of the other scatterplots. This is evidence against the hypothesis of interchangeability with $p = 1/20 = .05$, indicating a violation of the interchangeability assumption. In practice, we would produce many more than 19 correlation coefficients from the permutation distribution and we would not look at all the scatterplots, but it is instructive to see what a fair selection of scatterplots look like under the assumption of interchangeability. A plot of the exact null distribution is given in Figure 6.

6. CONCLUDING REMARKS

When dealing with bivariate observations that have identical marginals, the exchangeability within the pairs suggests a permutation set of 2^n scatterplots. Our proposal to choose a "representative" scatterplot as the one whose Pearson correlation is closest to an accepted measure of the intraclass correlation seems reasonable since practitioners are comfortable seeing scatterplots with associated values of r. The ICC from the ANOVA model, $\hat{\rho}_A$, has long been a widely accepted measure of ρ, but any reasonable measure could be used instead. The median value of r' from the permutation distribution of scatterplots may have some merit as a new estimator of ρ. The choice of Pearson's r to measure the interclass correlation in each of the 2^n scatterplots is somewhat arbitrary.

Other measures, such as Kendall's τ and Spearman's ρ, can easily be used if desired. The principle is the same, but the corresponding ICC is required, e.g., see Whitfield (1949) and Rothery (1979), respectively.

When collecting family data as described in the LDL–C example, there may be, and typically are, more than two siblings per family. In this case it is not obvious what (scatter) plot best graphically illustrates the meaning and magnitude of an ICC. An idea motivated by considering the one-way random effects model is the following. $\hat{\rho}_A$ is a function of the variance components associated with the family effect a_i and residual effect e_{ij}. The respective variation in these unobservable random effects provide the necessary elements to assess the between-family variation. Therefore, it is natural to conjecture that a plot involving the best linear unbiased predictors (BLUPs; Robinson, 1991) of these effects could be developed to graphically interpret the correlation coefficient. An approach in this direction appears promising.

Finally, the permutation distribution of the 2^n scatterplots suggests a test for the interchangeability of two paired variables. If the observed value of the interclass correlation is extreme, when compared to its value computed on each scatterplot in the permutation set, then we can reject the hypothesis of interchangeability.

APPENDIX: NOTATION AND PROOFS

Let (X_i, Y_i), $i = 1, \ldots, n$, be independent and identically distributed bivariate random variables, and let $(X_i', Y_i') = (X_i, Y_i)$ or (Y_i, X_i), i.e., either interchange of the X-Y labels within each pair, $i = 1, \ldots, n$. Define

$$r_s = \frac{\sum_{i=1}^{n}(X_i - \hat{\mu})(Y_i - \hat{\mu})}{\frac{1}{2}\left[\sum_{i=1}^{n}(X_i - \hat{\mu})^2 + \sum_{j=1}^{n}(Y_j - \hat{\mu})^2\right]}, \text{ where } \hat{\mu} = \frac{\bar{X} + \bar{Y}}{2},$$

and

$$r' = \frac{\sum_{i=1}^{n}(X_i' - \bar{X}')(Y_i' - \bar{Y}')}{\left[\sum_{i=1}^{n}(X_i' - \bar{X}')^2 \sum_{j=1}^{n}(Y_j' - \bar{Y}')^2\right]^{\frac{1}{2}}}, \text{ where } \bar{X}' = \frac{1}{n}\sum_{i=1}^{n}X_i' \text{ and } \bar{Y}' = \frac{1}{n}\sum_{i=1}^{n}Y_i'.$$

Lastly, define $r'_{min} = \min r'$, where the minimum is taken over all 2^n sets of $\{(X'_i, Y'_i) \mid i = 1,\ldots,n\}$.

Lemma. Let A and B be real numbers. Then $\left(\dfrac{A+B}{2}\right)^2 \geq AB$.

Proof. $\left(\dfrac{A+B}{2}\right)^2 = \dfrac{1}{4}\left[A^2 + 2AB + B^2\right] = \dfrac{1}{4}\left[A^2 - 2AB + B^2\right] + AB = \left(\dfrac{A-B}{2}\right)^2 + AB \geq AB.$

Note that if A and B are nonnegative, this is the familiar inequality between the arithmetic and geometric means.

Theorem. If $r'_{min} \geq 0$, then $r_s \leq r'_{min}$.

Proof. Note that the numerators of r_s and r'_{min} can be written as $\displaystyle\sum_{i=1}^{n} X_i Y_i - n\hat{\mu}^2$ and $\displaystyle\sum_{i=1}^{n} X_i Y_i - n\bar{X}'\bar{Y}'$,

respectively. From the *Lemma*,

$$\hat{\mu}^2 = \left(\frac{\bar{X}+\bar{Y}}{2}\right)^2 = \left(\frac{1}{2n}\sum_{i=1}^{n}(X_i + Y_i)\right)^2 = \left(\frac{1}{2n}\sum_{i=1}^{n}(X'_i + Y'_i)\right)^2 = \left(\frac{\bar{X}'+\bar{Y}'}{2}\right)^2 \geq \bar{X}'\bar{Y}'.$$

Hence,

$$\sum_{i=1}^{n} X_i Y_i - n\hat{\mu}^2 \leq \sum_{i=1}^{n} X_i Y_i - n\bar{X}'\bar{Y}'. \tag{2}$$

Properties of the sample mean and the *Lemma* give the following string of inequalities:

$$\frac{1}{2}\left[\sum_{i=1}^{n}(X_i - \hat{\mu})^2 + \sum_{j=1}^{n}(Y_j - \hat{\mu})^2\right] = \frac{1}{2}\left[\sum_{i=1}^{n}(X'_i - \hat{\mu})^2 + \sum_{j=1}^{n}(Y'_j - \hat{\mu})^2\right] \geq \frac{1}{2}\left[\sum_{i=1}^{n}(X'_i - \bar{X}')^2 + \sum_{j=1}^{n}(Y'_j - \bar{Y}')^2\right]$$

$$\geq \left[\sum_{i=1}^{n}(X'_i - \bar{X}')^2 \sum_{j=1}^{n}(Y'_j - \bar{Y}')^2\right]^{\frac{1}{2}}.$$

Combining this with (2) and the fact that $r'_{min} \geq 0$, we see that $r_s \leq r'_{min}$.

In the twin context positive correlation is the case of practical interest. If $r'_{min} < 0$, then we cannot be sure about its relationship to r_s. However, it does follow that $r_s < 0$ as well.

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Table 1. IQ measurements on five pairs of fraternal twins

Pair	IQs
1	(122, 118)
2	(102, 96)
3	(106, 99)
4	(116, 105)
5	(114, 99)

Table 2. Numbers of finger ridges on both hands of 12 pairs of female identical twins

Pair	No. of ridges	Pair	No. of ridges
1	(71, 71)	7	(114, 113)
2	(79, 82)	8	(57, 44)
3	(105, 99)	9	(114, 113)
4	(115, 114)	10	(94, 91)
5	(76, 70)	11	(75, 83)
6	(83, 82)	12	(76, 72)

Table 3. LDL cholesterol measurements on 31 pairs of brothers.

	Brother			Brother	
Family	Older	Younger	Family	Older	Younger
1	104	93	17	62	68
2	85	112	18	112	86
3	86	101	19	88	72
4	90	82	20	87	55
5	65	66	21	73	94
6	103	124	22	80	100
7	63	74	23	104	102
8	59	101	24	95	108
9	120	92	25	108	105
10	73	56	26	92	114
11	100	87	27	99	102
12	53	63	28	134	76
13	77	104	29	58	82
14	97	102	30	84	73
15	81	77	31	98	136
16	97	89			

Table 4. Measurements by two different observers of cardiac output of 23 patients

	Observer			Observer	
Patient	A	B	Patient	A	B
1	4.8	5.8	13	7.7	8.5
2	5.6	5.1	14	7.7	9.5
3	6.0	7.7	15	8.2	9.1
4	6.4	7.8	16	8.2	10.0
5	6.5	7.6	17	8.3	9.1
6	6.6	8.1	18	8.5	10.8
7	6.8	8.0	19	9.3	11.5
8	7.0	8.1	20	10.2	11.5
9	7.0	6.6	21	10.4	11.2
10	7.2	8.1	22	10.6	11.5
11	7.4	9.5	23	11.4	12.0
12	7.6	9.6			

Figure 1. 16 scatterplots and their correlations from the permutation distribution of the data in Table 1.

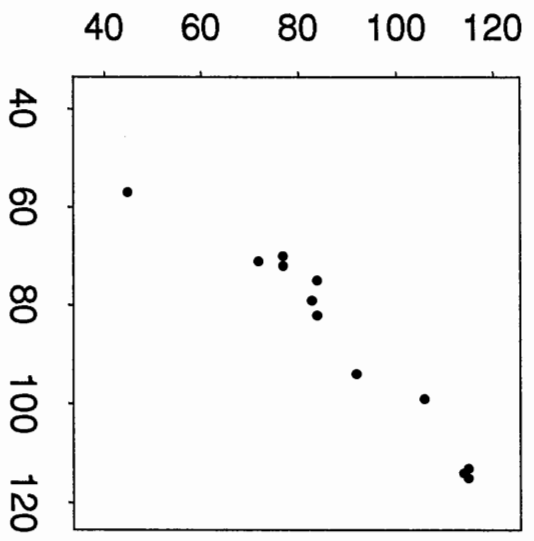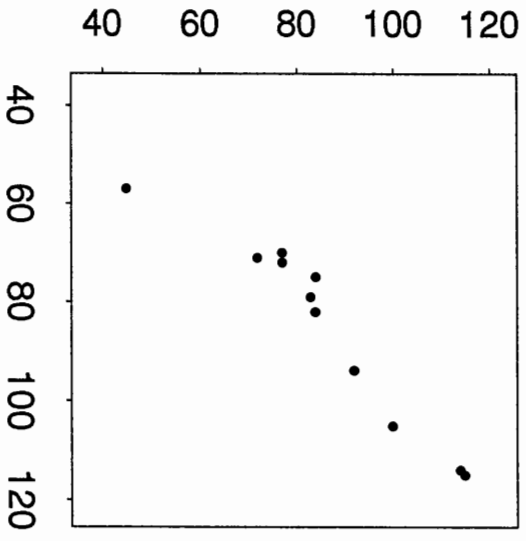*Figure 2. Histogram of the values of r' from the permutation distribution of the data in Table 2. The solid line marks $\hat{\rho}_A$ and the dashed line marks r_s.*

Figure 3. Four scatterplots from the permutation distribution of the data in Table 2. (a) Scatterplot with r' closest to $\hat{\rho}_A$. (b) Scatterplot with median r'. (c) Scatterplot with minimum r'. (d) Scatterplot with maximum r'.

Figure 4. Two scatterplots and a histogram from the permutation distribution of the LDL cholesterol data in Table 3. (a) Scatterplot with median r'. (b) Scatterplot with the Y value greater than the X value in each pair. (c) Histogram of the permutation distribution of r'.

Figure 5. Scatterplot of the data in Table 4 (upper left) and 19 randomly selected scatterplots from the permutation distribution with correlations.

Figure 6. Histogram of the values of r' from the permutation distribution of the data in Table 4.

0.587

0.507

0.424

0.414

0.628

0.507

0.424

0.414

0.739

0.508

0.437

0.42

0.867

0.512

0.497

0.421
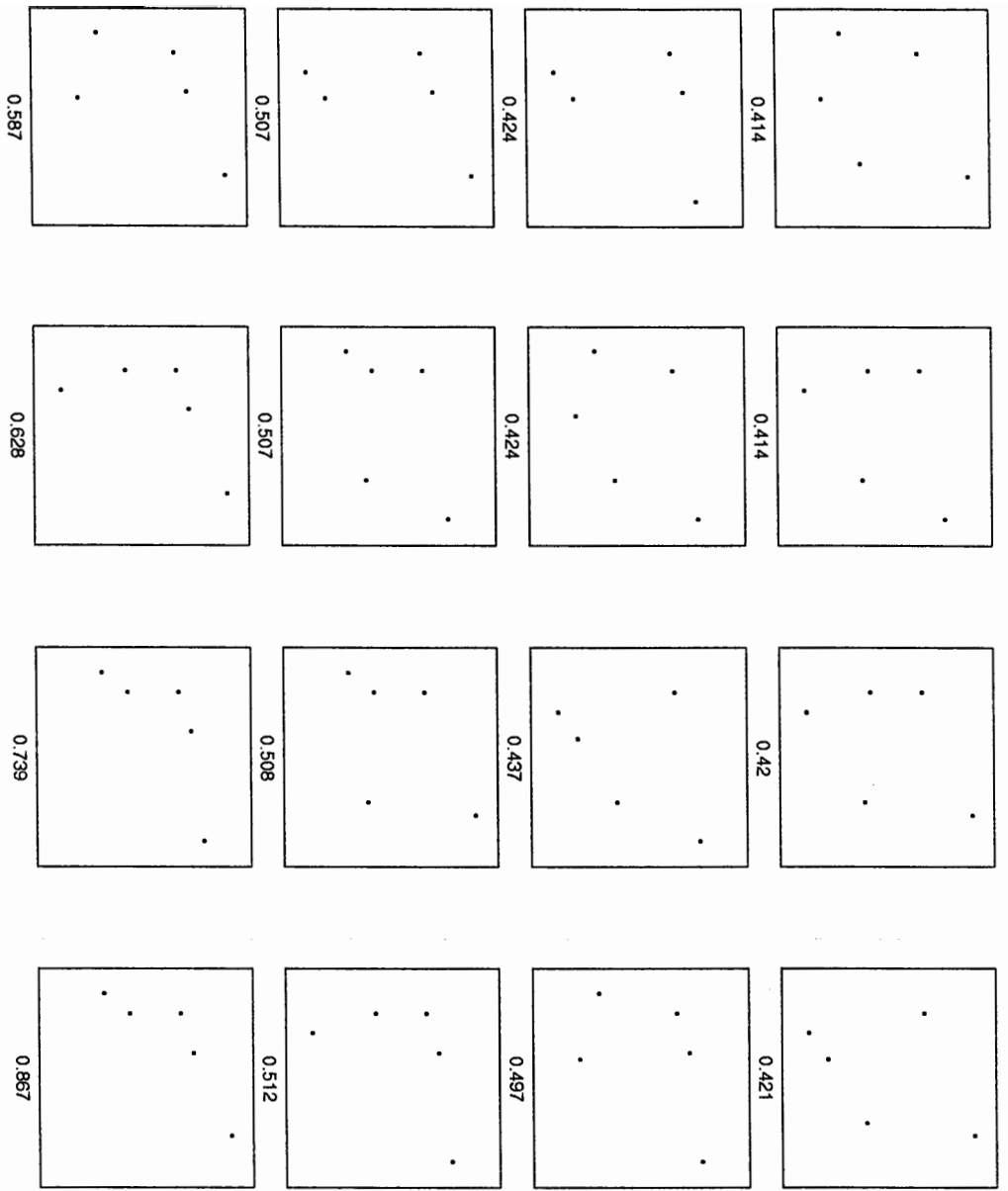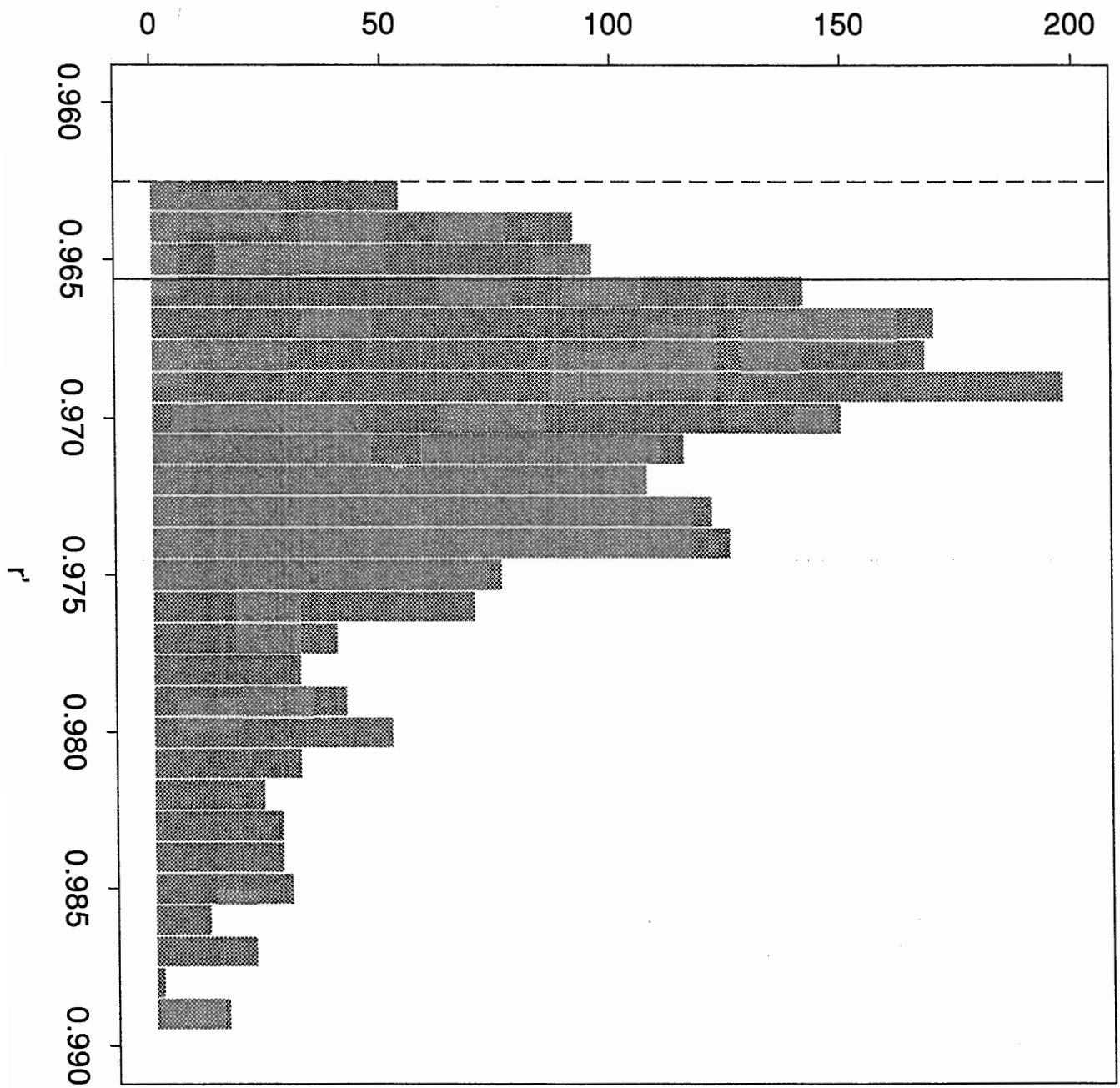
Figure 1

Figure 2

Plot with r' closest
to ANOVA estimate

(a) r = .9656

Plot with Minimum r'

(c) r = .9627
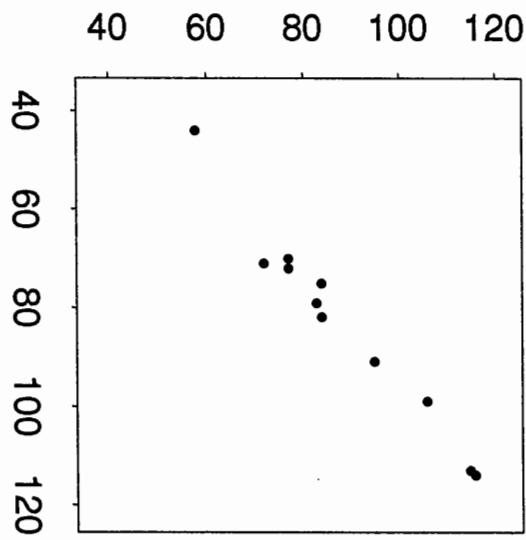
Plot with Median r'
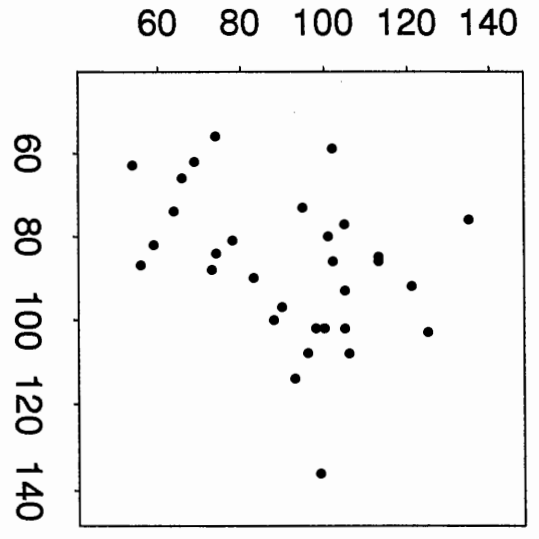
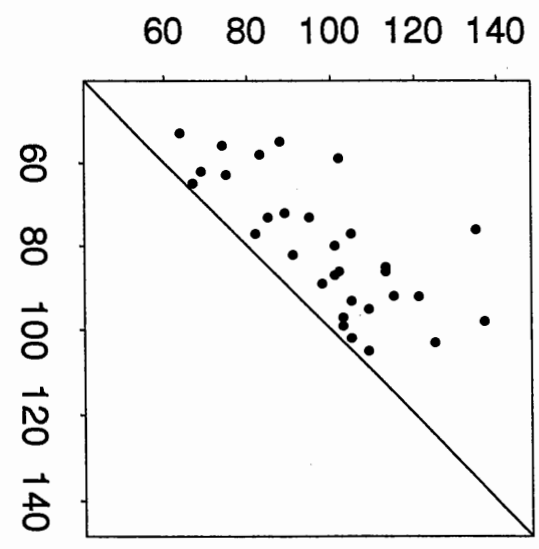(b) r = .9702

Plot with Maximum r'
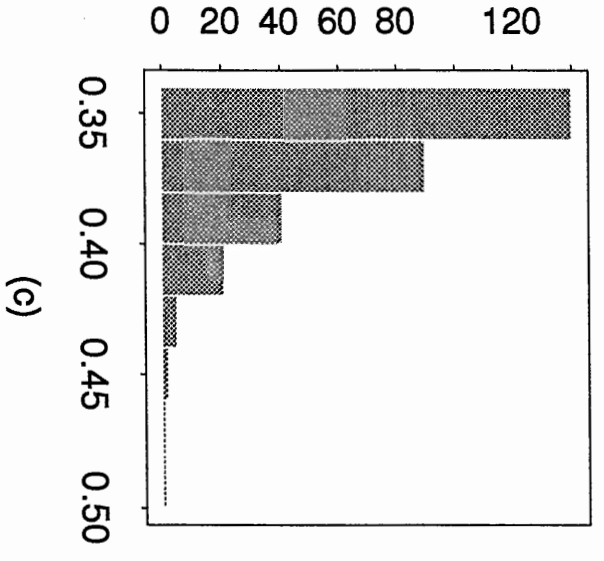
(d) r = .9890

Figure 3

Plot with Median r'

(a) r = .362

Plot with Y > X

(b) r = .719

301 sampled values of r'

(c)

Figure 4

Figure 5